

hep-ph/0403128

Subtraction Terms for Hadronic Production Processes at Next-to-Next-to-Leading Order

William B. Kilgore

*Physics Department, Brookhaven National Laboratory,
Upton, New York 11973, U.S.A.
[kilgore@bnl.gov]*

I describe a subtraction scheme for the next-to-next-to-leading order calculation of single inclusive production at hadron colliders. Such processes include Drell-Yan, W^\pm , Z and Higgs Boson production. The key to such a calculation is a treatment of initial state radiation which preserves the production characteristics, such as the rapidity distribution, of the process involved. The method builds upon the Dipole Formalism and, with proper modifications, could be applied to deep inelastic scattering and e^+e^- annihilation to hadrons.

PACS numbers: 14.70.-e, 14.80.Bn, 12.38.-t, 12.38.Bx

INTRODUCTION

Next-to-next-to-leading order (NNLO) calculations combine three contributions: Second order virtual corrections, first order virtual corrections to single real emission and double real emission. For special processes, like inclusive single particle production or inclusive deep inelastic scattering, fully inclusive NNLO calculations can be performed by analytically integrating over the total phase space [1–9]. In doing so, however, much of the exclusive information from the real emission processes is lost. In addition, it is difficult to impose geometric and kinematic cuts on the phase space that would correspond to a realistic experimental environment, although important progress within the framework of totally inclusive calculations has recently been made on this subject [10, 11]. Still, one would like to be able to perform a numerical calculation, valid to NNLO, which would retain the exclusive information of hard real emission and allow one to impose arbitrarily complicated cuts on the data.

The difficulty in constructing such a program is that each of the three contributions to the NNLO cross section is infrared divergent. It is only the sum of the three that yields a meaningful physical result. Combining the three terms is made difficult by the fact that each term involves a different number of final state particles and must therefore be integrated over a different phase space. Still, it should be possible to reorganize the infrared singularities, by adding and subtracting local counter-terms, so that one can perform and combine three *finite* calculations. Indeed, at next-to-leading order (NLO), the solution is well understood and a variety of methods have been successfully implemented.

A great deal of work has been devoted to the development of a general algorithm for constructing the local counter-terms at NNLO [12–17], but as yet there is no concrete example of a successful algorithm. Indeed the first successful “semi-inclusive” NNLO calculation was accomplished very recently [18], and did not use the analytic cancellation of in-

frared singularities afforded by a general subtraction method. Instead, it used the strategy of sector decomposition [19–23] to numerically cancel the singular contributions.

In this letter, I will describe an analytic subtraction scheme for the NNLO calculation of inclusive single particle production which builds upon the framework of the dipole formalism [24, 25]. In doing so, I do not solve the hardest problems associated with constructing a general purpose NNLO algorithm. Instead, I make use of the relative simplicity of the amplitudes involved and the control afforded by my ability to compute total integrals in each of the phase spaces.

THE BASIC FRAMEWORK AT NLO

I first review the basic framework for NLO calculations and build upon that to construct a solution at NNLO. An NLO calculation for an n parton cross section can be expressed as

$$\sigma^{\text{NLO}} = \int_{n+1} d\sigma_{n+1}^{(0)} + \int_n d\sigma_n^{(1)}, \quad (1)$$

where the subscripts refer to the number of final state particles for a particular term and the superscripts refer to the order in the α_s expansion to which the term is calculated. Because of the different numbers of particle in their phase spaces, the two calculations must be performed separately. The fact that both contributions are infrared divergent presents a non-trivial challenge to numerical calculations. A solution to this problem involves the construction of local counter-terms to the real emission cross section which permit a factorization of the phase space. The construction of such local counter-terms is made possible by the infrared factorization properties of QCD matrix elements. Introducing such terms, the NLO calculation now becomes

$$\begin{aligned} \sigma^{\text{NLO}} = & \int_{n+1} \left(d\sigma_{n+1}^{(0)} - d\alpha_{n+1}^{(0)} \right) \\ & + \int_n d\sigma_n^{(1)} + \int_{n+1} d\alpha_{n+1}^{(0)}, \end{aligned} \quad (2)$$

where $d\alpha_{n+1}^{(0)}$ is the local counter-term. $d\alpha_{n+1}^{(0)}$ is constructed such that it factorizes into the product of $d\sigma_n^{(0)}$, the n parton Born term, and an infrared singular term that can be completely integrated out of a factorization of $(n+1)$ -body phase space into n -body phase space times 1-body phase space. Thus, the terms on the first line in Eq. (2) are evaluated in the $(n+1)$ -body phase space, while those on the second line are evaluated in the n -body phase space.

When the radiative emission is hard, or rather, resolved, $d\alpha_{n+1}^{(0)}$ and $d\sigma_{n+1}^{(0)}$ map to different points in phase space and may be quite different in numerical value. When the emission is unresolved, however, the two terms map to the same point in phase space and their infrared singular terms cancel numerically. In the limit, the cancellation is complete and such terms do not contribute to the integral.

ON TO NNLO

In analogous fashion, an NNLO calculation is expressed as

$$\sigma^{\text{NNLO}} = \int_{n+2} d\sigma_{n+2}^{(0)} + \int_{n+1} d\sigma_{n+1}^{(1)} + \int_n d\sigma_n^{(2)}. \quad (3)$$

Again, each of the integrals on the right hand side is infrared divergent and again, one proceeds by constructing local counter-terms, but now the structure of the terms will be rather more complicated.

$$\begin{aligned} \sigma^{\text{NNLO}} = & \int_{n+2} \left(d\sigma_{n+2}^{(0)} - d\alpha_{n+2}^{(0)} + d\beta_{n+2}^{(0)} - d\gamma_{n+2}^{(0)} \right) \\ & + \int_{n+1} \left(d\sigma_{n+1}^{(1)} - d\alpha_{n+1}^{(1)} \right) + \int_{n+2} \left(d\alpha_{n+2}^{(0)} - d\beta_{n+2}^{(0)} \right) \\ & + \int_n d\sigma_n^{(2)} + \int_{n+1} d\alpha_{n+1}^{(1)} + \int_{n+2} d\gamma_{n+2}^{(0)}, \end{aligned} \quad (4)$$

where $d\alpha_{n+2}^{(0)}$ is the tree-level single real emission counter-term to $d\sigma_{n+2}^{(0)}$ like that found at NLO, $d\beta_{n+2}^{(0)}$ is a local counter-term to $d\alpha_{n+2}^{(0)}$ which cancels the singularities due to a subsequent second real emission, $d\gamma_{n+2}^{(0)}$ is the tree-level double real emission counter-term to $d\sigma_{n+2}^{(0)}$, and $d\alpha_{n+1}^{(1)}$ is the one-loop single real emission counter-term to $d\sigma_{n+1}^{(1)}$. As I have written Eq. (4), the terms on the first line are all computed in the $(n+2)$ -body phase space, the terms on the second line in $(n+1)$ -body phase space (after integrating out a single emission from $d\alpha_{n+2}^{(0)}$ and $d\beta_{n+2}^{(0)}$) and the terms on the third line are computed in n -body phase after integrating out the single and double emissions from $d\alpha_{n+1}^{(1)}$ and $d\gamma_{n+2}^{(0)}$ respectively.

It might seem that $d\beta_{n+2}^{(0)}$ could be constructed by iterating the procedure used to produce $d\alpha_{n+2}^{(0)}$. This is unlikely to work properly since only the infrared structure of each factorization is universal. The overlap of infrared singularities from one factorization with the finite remainder of the other is likely to generate spurious infrared divergences. Moreover

it is not necessary. One does not need a factorized approximation to $d\alpha_{n+2}^{(0)}$ since one does not need to integrate out the second emission to get down to the n -body phase space. Instead, one merely needs to know the locus in phase space that $d\alpha_{n+2}^{(0)}$ will map to under sequential emission. Thus, $d\beta_{n+2}^{(0)}$ should be made numerically identical to $d\alpha_{n+2}^{(0)}$ but should be evaluated at the point in phase space corresponding to the second emission.

The $d\gamma_{n+2}^{(0)}$ and $d\alpha_{n+1}^{(1)}$ counter-terms must approximate the soft and collinear limits of one-loop single real emission [26–28] and double real emission [29–33]. Recently, Weinzierl has reported a result for $d\alpha_{n+1}^{(1)}$ appropriate for one-loop final-state emission, which is the only case needed for the computation of $e^+e^- \rightarrow \text{jets}$ [16].

It would be possible to reformulate Weinzierl’s subtraction terms for case of initial state radiation required for the single particle production processes considered here, but that is not the solution that I propose. Instead, I use the same strategy in constructing $d\gamma_{n+2}^{(0)}$ and $d\alpha_{n+1}^{(1)}$ as I used for constructing $d\beta_{n+2}^{(0)}$: rather than constructing approximations to the matrix element at some point in phase space, I use the exact matrix elements but evaluate them as if they were at different point in phase space. I can do this because I have complete analytic control of the total integrals of these matrix elements over phase space.

With this strategy, it is clear that if I compute the total rate, placing no kinematic or geometric cuts on the configuration and not binning any distributions, the first two lines in Eq. (4) vanish identically, while the third line gives the known result for the inclusive cross section.

RAPIDITY DISTRIBUTIONS

The simple framework described above is sufficient for describing the total rate, but does not include all of the information available in inclusive production. In addition to the total rate, one can also observe the rapidity distributions of the vector or Higgs boson [10, 11]. In order to reproduce rapidity distributions in this calculation, one needs rapidity information in the subtraction term. The subtraction term in the full $(n+2)$ -body phase space certainly contains this information. What is needed is a means of capturing this information in the n -body phase space. The way to do so is to understand the structure of the subtraction term in the n -body phase space: in final state emission, the subtraction term in the n -body phase space is essentially a number; in initial state emission, it is a convolution of the emission contributions with the partonic cross section and can be expressed in a form reminiscent of mass factorization,

$$\sigma_{n+2-m}^{(m)} = \sum_{k=0}^m \sum_{j=0}^{2-k-m} \sigma_n^{(k)} \otimes \tilde{\Gamma}_1^{(j)} \otimes \tilde{\Gamma}_2^{(2-j-k-m)}, \quad (5)$$

where the superscripts refer to the order in the expansion in α_s of each term.

Unlike mass factorization, which relates the (infrared singular) contributions determined by sum of squared matrix elements integrated over phase space to a convolution of finite partonic cross section with the mass factorization counter-terms associated with the Altarelli-Parisi splitting functions, Eq. (5) seeks to relate individual components, say $q\bar{q} \rightarrow Vgg$, to a convolution of the virtual cross section, evaluated to the appropriate order, with real emission counter-terms. The “appropriate order” is determined by the factorization properties of the QCD matrix elements. Specifically, double real radiation terms map onto a convolution of the virtual term at Born level with either two single emission terms or one double emission term, while one-loop single real radiation terms map onto the sum of the one-loop virtual term convolved with one first-order single emission term and the Born level virtual term convolved with one second-order single emission term.

To be more explicit, I will consider vector boson production and define the mass of the vector boson to be M_V and the center-of-mass (c.m.) energy squared of the production process to be \hat{s} . The ratio of the vector boson mass squared to \hat{s} is defined to be $z \equiv M_V^2/\hat{s}$, the momentum fractions of the incoming partons are defined to be x_1 and x_2 ($\hat{s} = x_1 x_2 s$), and the fraction of those momentum fractions that go into vector boson production are defined to be w_1 and w_2 ($z = w_1 w_2$). In terms of these parameters,

$$\begin{aligned} d\hat{\sigma}_n(z) &= \delta(1-z) \left(a_0 + \frac{\alpha_s}{\pi} a_1 + \left(\frac{\alpha_s}{\pi} \right)^2 a_2 \right), \\ \tilde{\Gamma}_i(w_i) &= \delta(1-w_i) + \frac{\alpha_s}{\pi} \tilde{\Gamma}_i^{(1)}(w_i) + \left(\frac{\alpha_s}{\pi} \right)^2 \tilde{\Gamma}_i^{(2)}(w_i). \end{aligned} \quad (6)$$

In the virtual terms, all of the energy goes into vector boson production and the vector boson rapidity is identical to the rapidity of the lab system.

$$y_n = \frac{1}{2} \ln \frac{x_1}{x_2}. \quad (7)$$

In the case of single real radiation, some of the c.m. energy goes into vector boson production, but some goes into a single collinear emission. The convolution consists of terms for which the emission is in the direction of parton 1 and terms for which it is in the direction of parton 2. Given the energy and boost of the c.m. system, the mass of the vector boson and the direction of the radiative emission, it is a simple exercise to determine the rapidity of the vector boson:

$$y_{n+1} = \frac{1}{2} \ln \frac{x_1}{x_2} \pm \frac{1}{2} \ln z. \quad (8)$$

In an actual calculation, one generates vector bosons at a given rapidity and then convolves the parton distributions over the parton momentum fractions, using $\tilde{\Gamma}$ to properly weight the contributions above threshold.

Things are more complicated when one must consider double emission. In the triple collinear limit, where both emissions come from the same incoming leg, the kinematics is unchanged from the single emission case and one can determine

the rapidity of the vector boson from the direction of the emission. The case of overlapping emission, where each incoming parton contributes to the radiation is more complicated. In order to determine the rapidity of the vector boson, one needs to know what fraction of the radiation came from each side. Thus, for given parton momentum fractions x_1, x_2 , rather than generating vector bosons at distinct rapidities, as in Eq. (8), one generates them over a continuum of rapidities:

$$\begin{aligned} y_{n+2} &= \frac{1}{2} \ln \frac{x_1 w_1}{x_2 w_2}, \\ \frac{1}{2} \ln \frac{x_1}{x_2} + \frac{1}{2} \ln z &\leq y_{n+2} \leq \frac{1}{2} \ln \frac{x_1}{x_2} - \frac{1}{2} \ln z. \end{aligned} \quad (9)$$

Again, one generates vector bosons of a given rapidity and then convolves the parton distributions over the momentum fractions using $\tilde{\Gamma}$ to properly weight the contributions above threshold, but now one needs to know the appropriate $\tilde{\Gamma}_i$ on each side. The total integral over double emission phase space does not give $\tilde{\Gamma}_i$, however, it gives the second order contribution to the convolution

$$\tilde{\Gamma}^{(2)}(z) = \tilde{\Gamma}_1^{(2)}(z) + \tilde{\Gamma}_2^{(2)}(z) + \tilde{\Gamma}_1^{(1)}(w_1) \otimes \tilde{\Gamma}_2^{(1)}(w_2). \quad (10)$$

The terms $\tilde{\Gamma}_i^{(2)}$ correspond to the triple collinear limits of the incoming partons. Subtracting these terms off, one is left with just the overlapping emission term, each component of which can be expanded as a Laurent series in ϵ ,

$$\begin{aligned} \tilde{\Gamma}_{\text{overlap}}^{(2)} &= \tilde{\Gamma}_1^{(1)} \otimes \tilde{\Gamma}_2^{(1)}, \\ \tilde{\Gamma}_{\text{overlap}}^{(2)} &= \frac{g(-4)}{\epsilon^4} + \frac{g(-3)}{\epsilon^3} + \frac{g(-2)}{\epsilon^2} + \frac{g(-1)}{\epsilon} + g(0) + \dots, \\ \tilde{\Gamma}_i^{(1)} &= \frac{a_{i,(-2)}}{\epsilon^2} + \frac{a_{i,(-1)}}{\epsilon} + a_{i,(0)} + \epsilon a_{i,(1)} + \epsilon^2 a_{i,(2)} + \dots \end{aligned} \quad (11)$$

Since the infrared structure of single emission is universal, the most singular terms in Eq. (11) are fixed and the less singular terms can be solved for, term by term. When single emission is considered in isolation, the nonsingular terms, $a_{i,n \geq 0}$, are non-universal. In the context of overlapping divergences from double emission, however, these terms can be given meaningful definitions.

$$\begin{aligned} g(-4) &= a_{1,(-2)} \otimes a_{2,(-2)}, \\ g(-3) &= a_{1,(-1)} \otimes a_{2,(-2)} + a_{1,(-2)} \otimes a_{2,(-1)}, \\ g(-2) &= a_{1,(0)} \otimes a_{2,(-2)} + a_{1,(-2)} \otimes a_{2,(0)} \\ &\quad + a_{1,(-1)} \otimes a_{2,(-1)}, \\ g(-1) &= a_{1,(1)} \otimes a_{2,(-2)} + a_{1,(-2)} \otimes a_{2,(1)} \\ &\quad + a_{1,(0)} \otimes a_{2,(-1)} + a_{1,(-1)} \otimes a_{2,(0)}, \\ g(0) &= a_{1,(2)} \otimes a_{2,(-2)} + a_{1,(-2)} \otimes a_{2,(2)} \\ &\quad + a_{1,(1)} \otimes a_{2,(-1)} + a_{1,(-1)} \otimes a_{2,(-1)} \\ &\quad + a_{1,(0)} \otimes a_{2,(0)}, \end{aligned} \quad (12)$$

The singular terms must cancel against other infrared contributions, so all components involved in those terms can be de-

terminated unambiguously. While the soft contributions (corresponding to delta functions in the parton fractions) cannot be uniquely distributed among the separate terms, their distribution does not affect the magnitude of the total subtraction nor its location in phase space. The only room for ambiguity would come in the terms that are new to $g_{(0)}$, *i.e.* $a_{1,(2)}$ and $a_{2,(2)}$. When the splittings are symmetric, say for $q\bar{q} \rightarrow Vgg$ each splitting would be $q \rightarrow \tilde{q}g$ (where \tilde{a} identifies the incoming parton), the solution is symmetric and there is no ambiguity. When the splittings are asymmetric, say for $qg \rightarrow Vqg$ where one splitting is $q \rightarrow \tilde{q}g$ and the other is $q \rightarrow \check{q}g$ (note the order), it may seem that one cannot separate the new terms. However, the prior knowledge of the more singular terms with which they are convolved should allow for this extraction. Certainly the dominant terms can be determined unambiguously. It is also possible to obtain rapidity distributions at NNLO within the framework of inclusive calculations and this has already been done for Drell-Yan production [11]. The information from such a calculation could be used to resolve any lingering ambiguities.

Implicit to the preceding discussion is that the $d\gamma_{n+2}^{(0)}$ and $d\alpha_{n+1}^{(1)}$ in the $(n+2)$ and $(n+1)$ -body phase spaces must be evaluated at points in phase space that correspond to those described in n -body phase space. Those points correspond to conserving the incoming parton momentum fractions of the true process, but mapping all final state momenta onto the beam axes. In the event of unresolved emission, this mapping ensures a proper subtraction of the singularities.

CONCLUSIONS

In this letter, I have described the explicit construction of the subtraction terms needed for an NNLO parton-level monte carlo calculation of single inclusive production (Higgs bosons, vector bosons, Drell-Yan) within the dipole formalism. For these simple processes, one has complete analytic control over the total integrals of the matrix elements. This control allows one to use the matrix elements themselves as the subtraction terms. In order to capture the full information available from inclusive calculations, one needs to retain information on both the total rate and the rapidity distribution of production. I have outlined a method for doing so.

Acknowledgments: I would like to thank Michelangelo Mangano for emphasizing the importance of this project. I would also like to thank the Kavli Institute for Theoretical Physics, where part of this work was done, for their kind hospitality. This research was supported in part by the National Science Foundation under Grant No. PHY99-07949 and in part by the U. S. Department of Energy under Contract No. DE-AC02-98CH10886.

Note: As this paper was being completed, I became aware of Ref. [34], in which essentially the same solution is proposed for the final state emission process, $e^+e^- \rightarrow 2$ jets, and is worked out in great detail.

-
- [1] R. Hamberg, W. L. van Neerven, and T. Matsuura, Nucl. Phys. **B359**, 343 (1991).
 - [2] W. L. van Neerven and E. B. Zijlstra, Phys. Lett. **B272**, 127 (1991).
 - [3] R. V. Harlander and W. B. Kilgore, Phys. Rev. Lett. **88**, 201801 (2002), hep-ph/0201206.
 - [4] C. Anastasiou and K. Melnikov, Nucl. Phys. **B646**, 220 (2002), hep-ph/0207004.
 - [5] R. V. Harlander and W. B. Kilgore, JHEP **10**, 017 (2002), hep-ph/0208096.
 - [6] C. Anastasiou and K. Melnikov, Phys. Rev. **D67**, 037501 (2003), hep-ph/0208115.
 - [7] V. Ravindran, J. Smith, and W. L. van Neerven, Nucl. Phys. **B665**, 325 (2003), hep-ph/0302135.
 - [8] R. V. Harlander and W. B. Kilgore, Phys. Rev. **D68**, 013001 (2003), hep-ph/0304035.
 - [9] V. Ravindran, J. Smith, and W. L. van Neerven (2003), hep-ph/0311304.
 - [10] C. Anastasiou, L. J. Dixon, K. Melnikov, and F. Petriello, Phys. Rev. Lett. **91**, 182002 (2003), hep-ph/0306192.
 - [11] C. Anastasiou, L. Dixon, K. Melnikov, and F. Petriello (2003), hep-ph/0312266.
 - [12] D. A. Kosower, Phys. Rev. **D67**, 116003 (2003), hep-ph/0212097.
 - [13] D. A. Kosower, Phys. Rev. Lett. **91**, 061602 (2003), hep-ph/0301069.
 - [14] D. A. Kosower (2003), hep-ph/0311272.
 - [15] S. Weinzierl, JHEP **03**, 062 (2003), hep-ph/0302180.
 - [16] S. Weinzierl, JHEP **07**, 052 (2003), hep-ph/0306248.
 - [17] S. Weinzierl (2003), hep-ph/0310164.
 - [18] C. Anastasiou, K. Melnikov, and F. Petriello (2004), hep-ph/0402280.
 - [19] T. Binoth and G. Heinrich, Nucl. Phys. **B585**, 741 (2000), hep-ph/0004013.
 - [20] T. Binoth and G. Heinrich, Nucl. Phys. **B680**, 375 (2004), hep-ph/0305234.
 - [21] A. Gehrmann-De Ridder, T. Gehrmann, and G. Heinrich (2003), hep-ph/0311276.
 - [22] C. Anastasiou, K. Melnikov, and F. Petriello (2003), hep-ph/0311311.
 - [23] T. Binoth and G. Heinrich (2004), hep-ph/0402265.
 - [24] S. Catani and M. H. Seymour, Phys. Lett. **B378**, 287 (1996), hep-ph/9602277.
 - [25] S. Catani and M. H. Seymour, Nucl. Phys. **B485**, 291 (1997), hep-ph/9605323.
 - [26] D. A. Kosower and P. Uwer, Nucl. Phys. **B563**, 477 (1999), hep-ph/9903515.
 - [27] S. Catani and M. Grazzini, Nucl. Phys. **B591**, 435 (2000), hep-ph/0007142.
 - [28] Z. Bern, V. Del Duca, W. B. Kilgore, and C. R. Schmidt, Phys. Rev. **D60**, 116001 (1999), hep-ph/9903516.
 - [29] F. A. Berends and W. T. Giele, Nucl. Phys. **B313**, 595 (1989).
 - [30] S. Catani (1992), report ETH-TH-93-01.
 - [31] J. M. Campbell and E. W. N. Glover, Nucl. Phys. **B527**, 264 (1998), hep-ph/9710255.
 - [32] S. Catani and M. Grazzini, Phys. Lett. **B446**, 143 (1999), hep-ph/9810389.
 - [33] S. Catani and M. Grazzini, Nucl. Phys. **B570**, 287 (2000), hep-ph/9908523.
 - [34] A. Gehrmann-De Ridder, T. Gehrmann, and E. W. N. Glover (2004), hep-ph/0403057.